

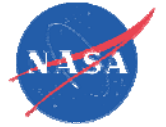


# Assessment of the National Combustion Code

Nan-Suey Liu, NASA GRC  
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Tsan-Hsing Shih, Ohio Aerospace Institute

## ABSTRACT

The advancements made during the last decade in the areas of combustion modeling, numerical simulation, and computing platform have greatly facilitated the use of CFD based tools in the development of combustion technology. Further development of verification, validation and uncertainty quantification will have profound impact on the reliability and utility of these CFD based tools. The objectives of the present effort are to establish baseline for the National Combustion Code (NCC) and experimental data, as well as to document current capabilities and identify gaps for further improvements.



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## Relationship to the Fundamental Aeronautics Program

- Project            Subsonic Fixed Wing
- Discipline        Combustion
- Element           Combustion Technologies & Tool Development
- Task                Combustion CFD Code Development and Application for Emissions and Flow Field Predictions



# Assessment of NCC for Emissions and Flow Field ( SFW 12.03.01)

## Background

- Advancements made during the last decade in the areas of combustion modeling, numerical simulation, and computing platform have greatly facilitated the use of combustion Computational Fluid Dynamics (CFD) in the development of combustion technology.
- Further development of verification, validation and uncertainty quantification will have a profound impact on the reliability and utility of modeling and simulation tools.
- In the mean time, significant improvements are still needed, not just in the areas of numerical accuracy and model fidelity, but also in the areas of analysis turnaround time ( in terms of the wall-clock time) and the costs.



# Assessment of NCC for Emissions and Flow Field ( SFW 12.03.01)

## Ultimate Goal

Through the development, validation and application of the National Combustion Code, and collaborate with NRA partners :

- To push the state-of-the-art in comprehensive combustion modeling and simulation;
- To provide quantitative information accompanied with estimated uncertainty in a reliable, timely, and cost effective manner;
- To establish an integrated approach using combustion CFD, diagnostics, and rig testing to advance the combustion technology.



# Assessment of NCC for Emissions and Flow Field ( SFW 12.03.01)

## Objectives

- Establish baseline for prediction methods and experimental data for lean direct injection (LDI) combustion in confined, swirling flows.
- Document current capabilities and identify gaps for future research.
- Improve prediction capabilities for emissions and performance of combustors using combustion CFD simulations.



# Assessment of NCC for Emissions and Flow Field ( SFW 12.03.01)

## Approach

- Assess baseline NCC (version 1.1.8).
- Incorporate partially resolved numerical simulation (PRNS) approach for very large eddy simulation (VLES) into NCC.
- Incorporate advanced physics-based models into NCC including models for turbulence-chemistry interaction, primary atomization and secondary breakup, and chemical kinetics.
- Incorporate NRA developed physics-based models into NCC as they become available and are appropriate.
- Gather experimental data suitable for model validation.
- Perform validation calculations and quantify the uncertainties of the models.
- Periodically assess the status of modeling & simulation and experimental data.



## Milestone Status ( SFW 12.03.01)

Milestones	Completion Date	Status
Perform steady RANS non-reacting flow calculations using NCC 1.1.8 for single LDI element data reported in AIAA-2005-1424	4/2007	Completed
Perform steady RANS liquid fueled reacting flow calculations using NCC 1.1.8 for single LDI element data reported in AIAA-2005-1424	9/2007	In progress
Perform VLES for turbulent pipe flow using the PRNS approach implemented in the NCC 1.1.8	9/2007	In progress
Documentation NCC assessment report for VLES capability NCC assessment report for single element LDI	12/2007	

### Major Issues

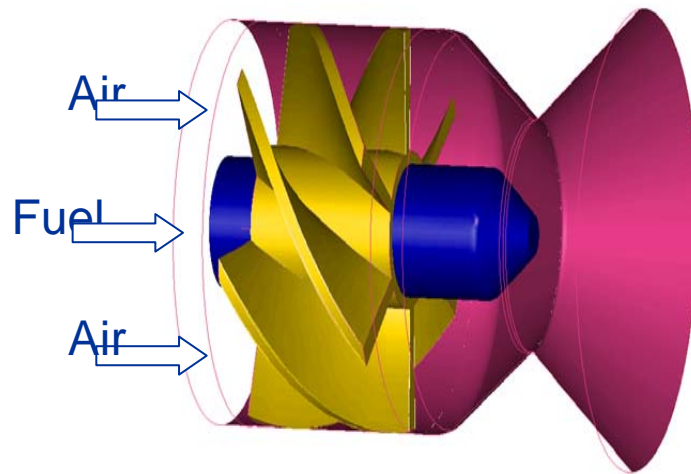
Meaningful and efficient approaches to the quantification of uncertainties and assessment of modeling & simulation credibility are yet to be established.

Assessing uncertainty/error costs at least as much as obtaining the answer in the first place.

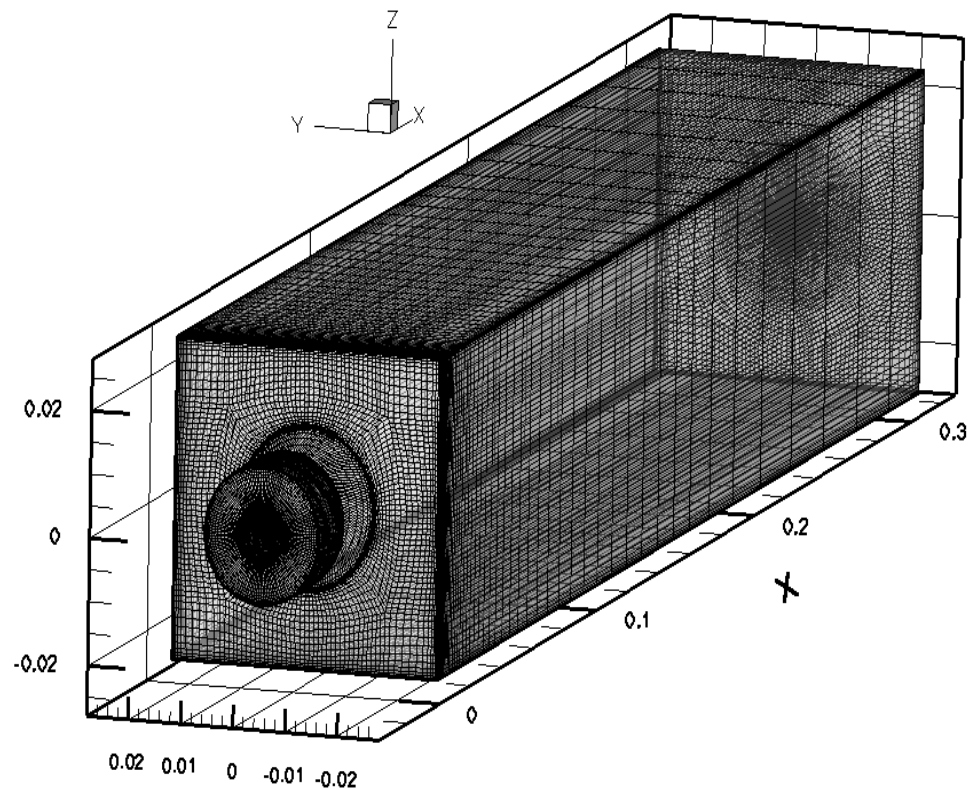




# The Structure of a Swirl-Stabilized Reacting Spray Issued from an Axial Swirler (Cai et al. AIAA-2005- 1424)



Geometry of the Single Element



Grid Distribution for the LDI Combustor (861823 hexahedron elements)

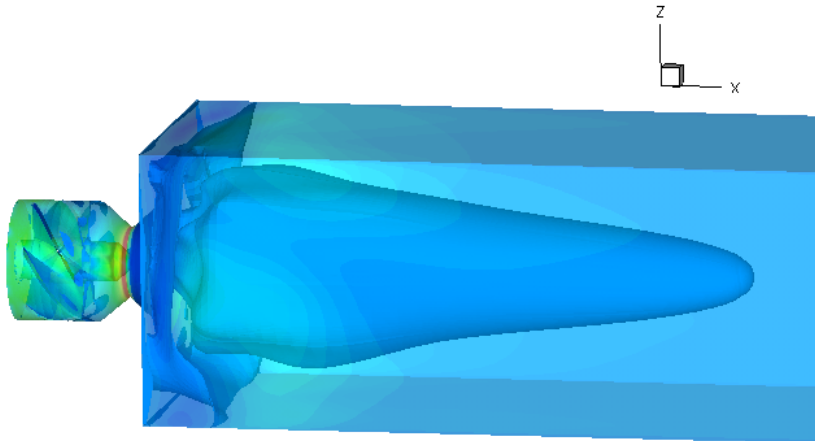


## Experimental Setup

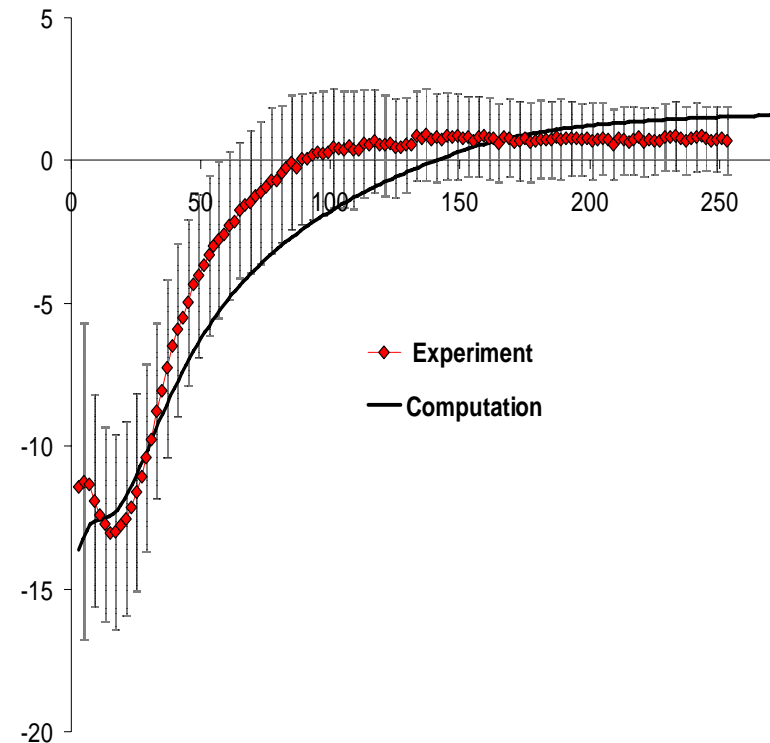
- The air swirler has six helical, axial vanes with downstream vane angle of 60 degrees.
- At the down stream of the swirler, a convergent-divergent venturi is attached to the swirler.
- At the exit of the venturi, a rectangular combustion chamber is attached.
- The fuel nozzle is a PARKER 90 degree, hollow cone, pressure swirl atomizer.
- Jet-A fuel is used as liquid fuel. The air mass flow rate is 0.49 kg/min and the fuel flow rate is 0.0249 kg/min, hence, the equivalence ratio is 0.75. The pressure difference between the air supply manifold and environment is 4% of atmospheric pressure.



## Non-reacting flow calculation



Iso-surface of zero axial velocity

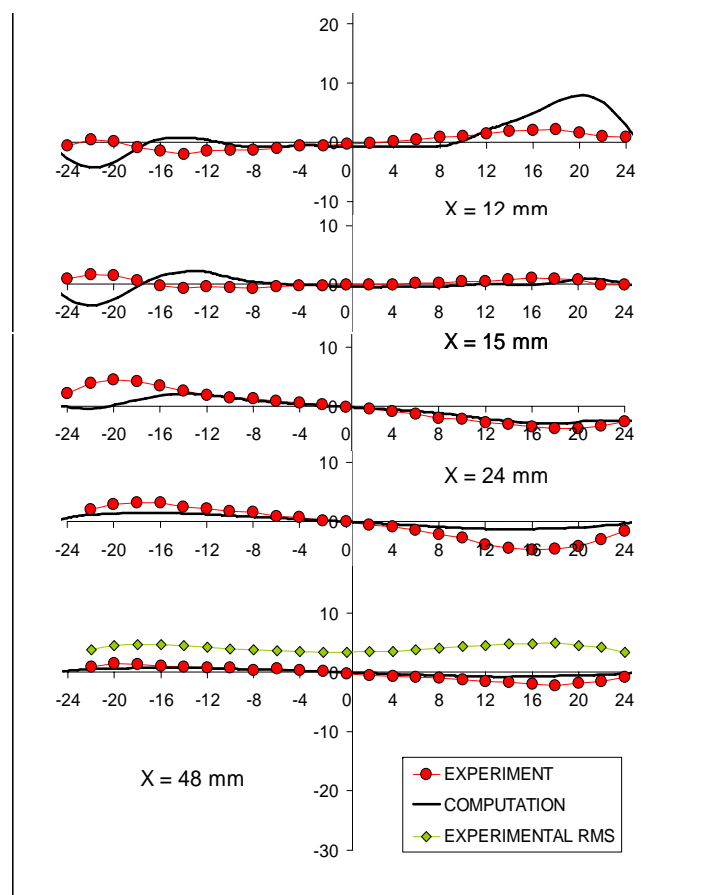
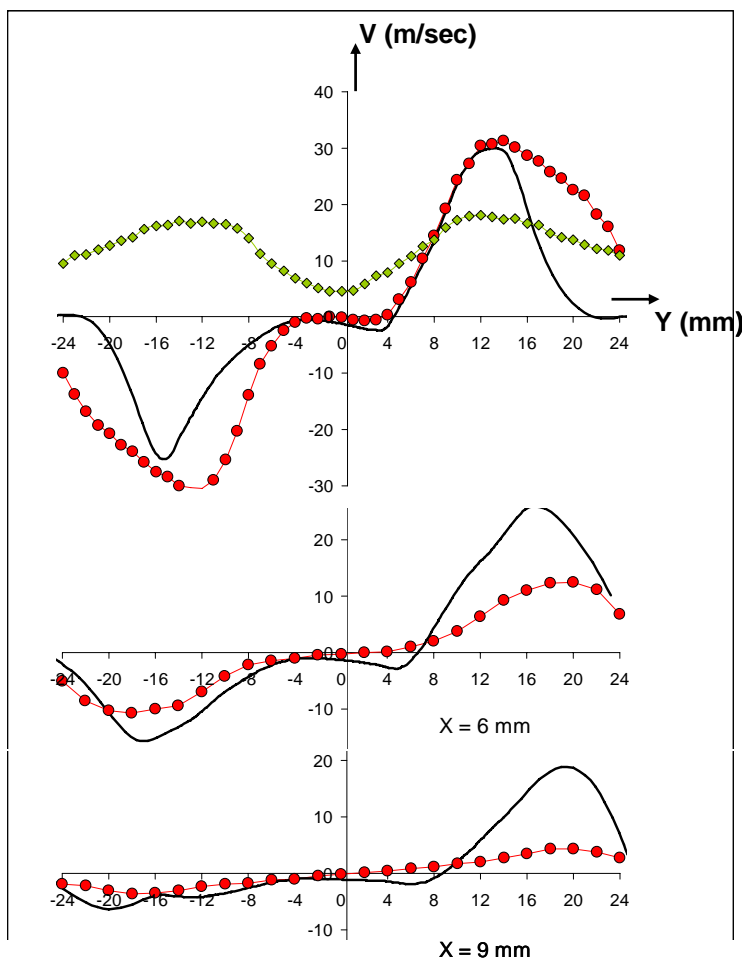


Axial velocity along the center line

The rms value of the experimental data is used to indicate the level of the large-scale unsteadiness of the flow



# Non-reacting flow calculation



Radial-velocity at different axial stations



## Spray Model

- The continuous annular sheet injection is computationally represented by a finite number of point injectors located within a circular ring very close to the fuel injector tip. During the injection process, the locations of these point injectors are fixed.
- Each point injector has an assumed drop-size distribution which is further represented by a finite number of droplet groups. Associated droplet diameters and velocities must also be specified.
- Experimental data are used to guide the specification of model parameters.



# Chemistry Models

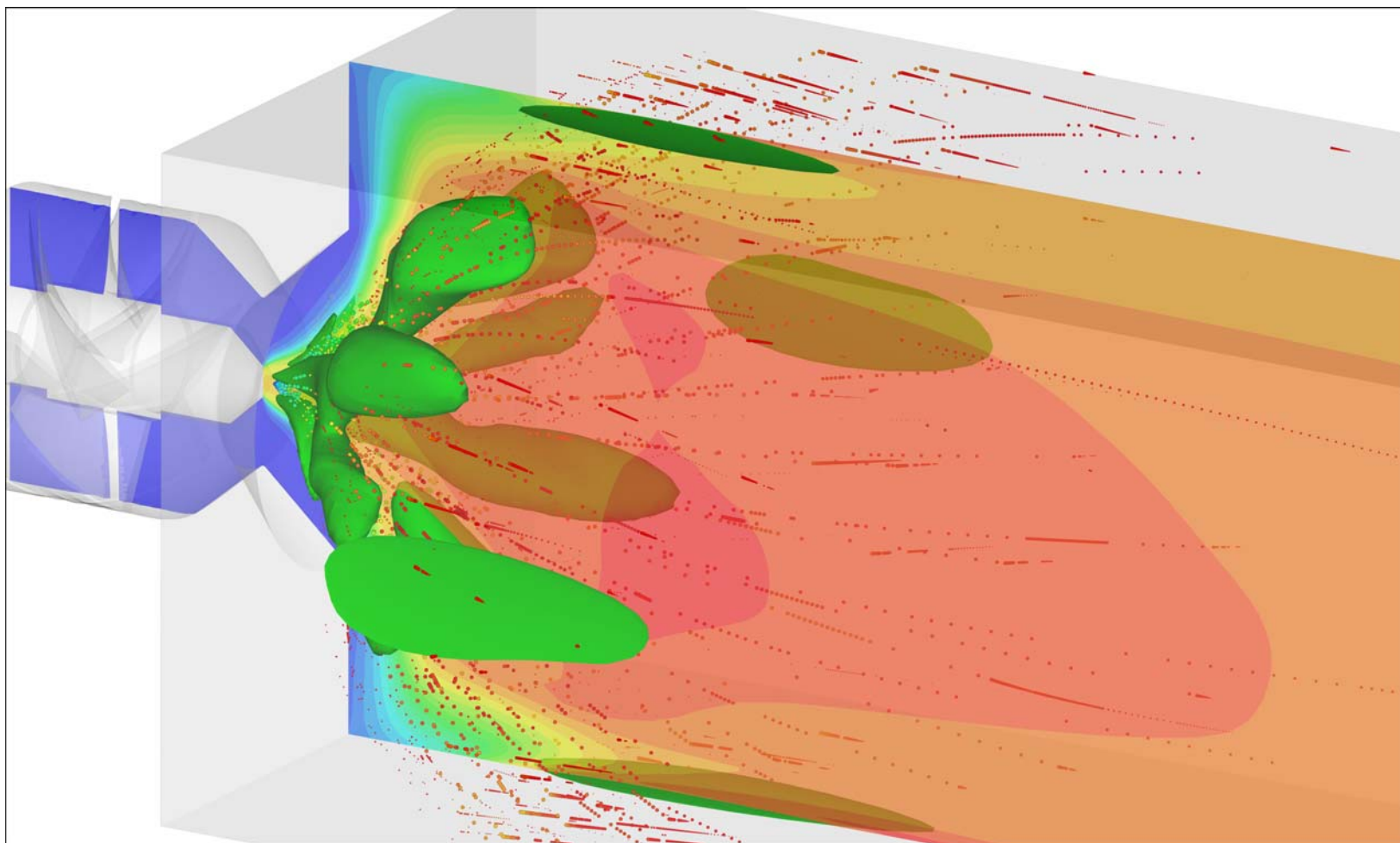
- One Step Model (5 species)  
 $4\text{C}_{12}\text{H}_{23} + 71\text{O}_2 \Rightarrow 48\text{CO}_2 + 46\text{H}_2\text{O}$

- Ten Step Model (12 species)  
 $4\text{C}_{12}\text{H}_{23} + 47\text{O}_2 \Rightarrow 48\text{CO} + 46\text{H}_2\text{O}$





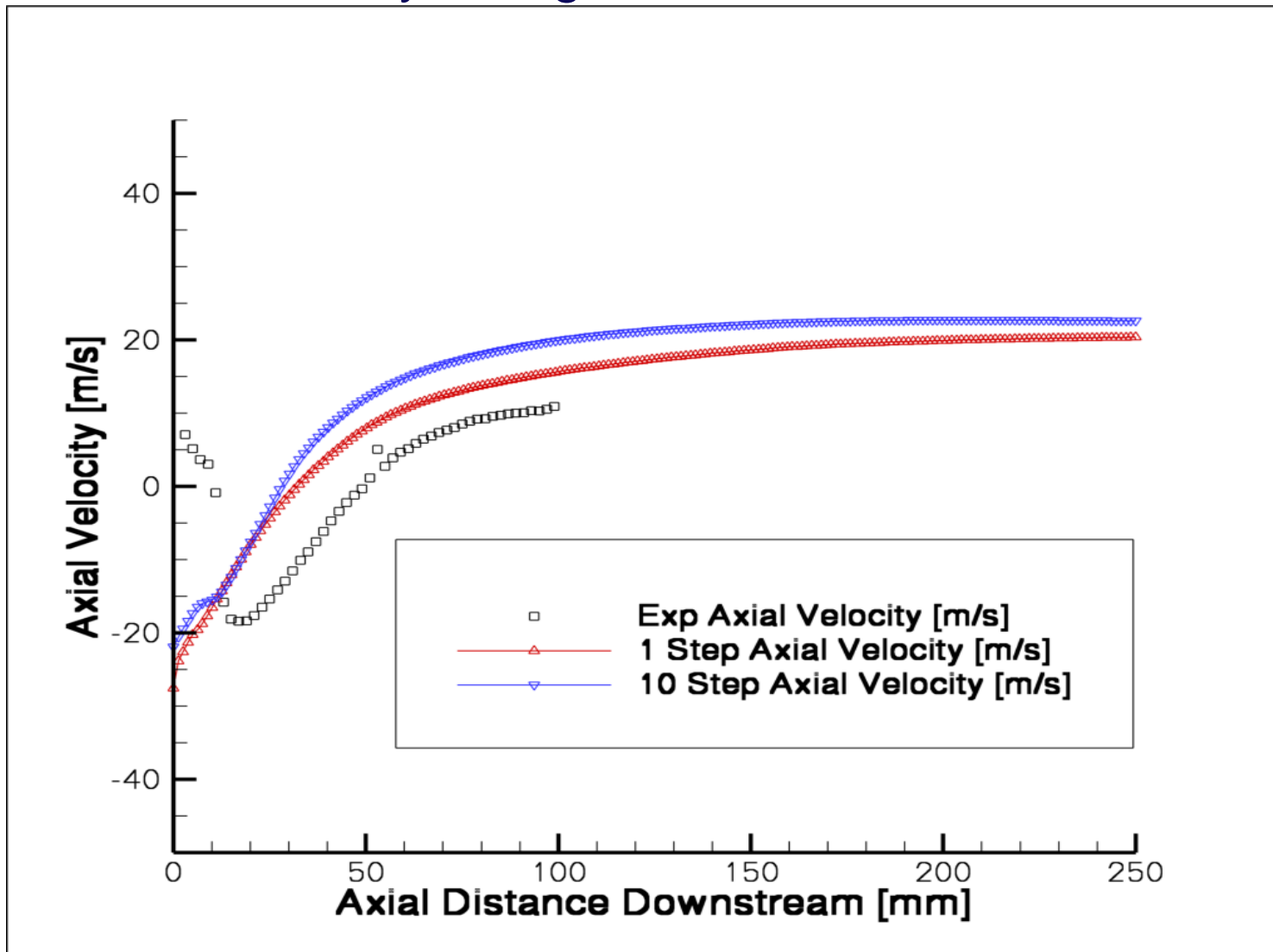
## Single Element Lean Direct Injection (LDI) Combustor Physical Processes Overview (Results obtained by using the 10-step chemistry model)







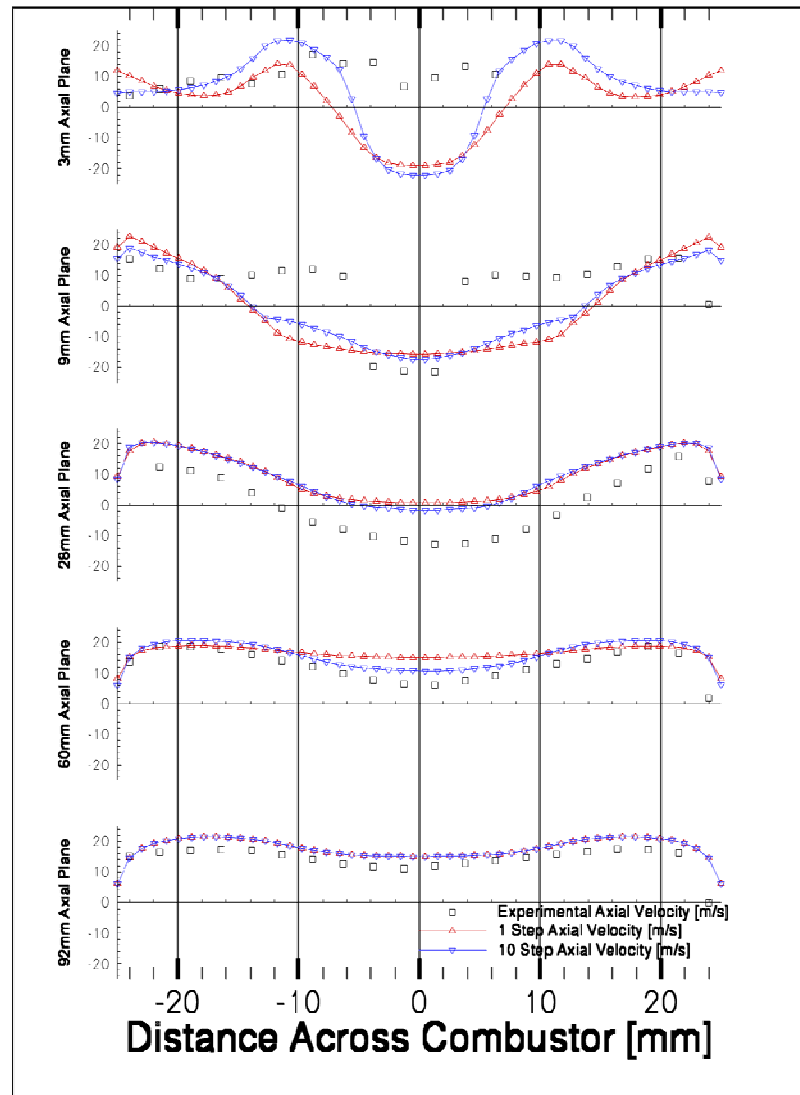
## Reacting Spray Flow, Comparison of Mean Axial Velocity Along the Axial Centerline





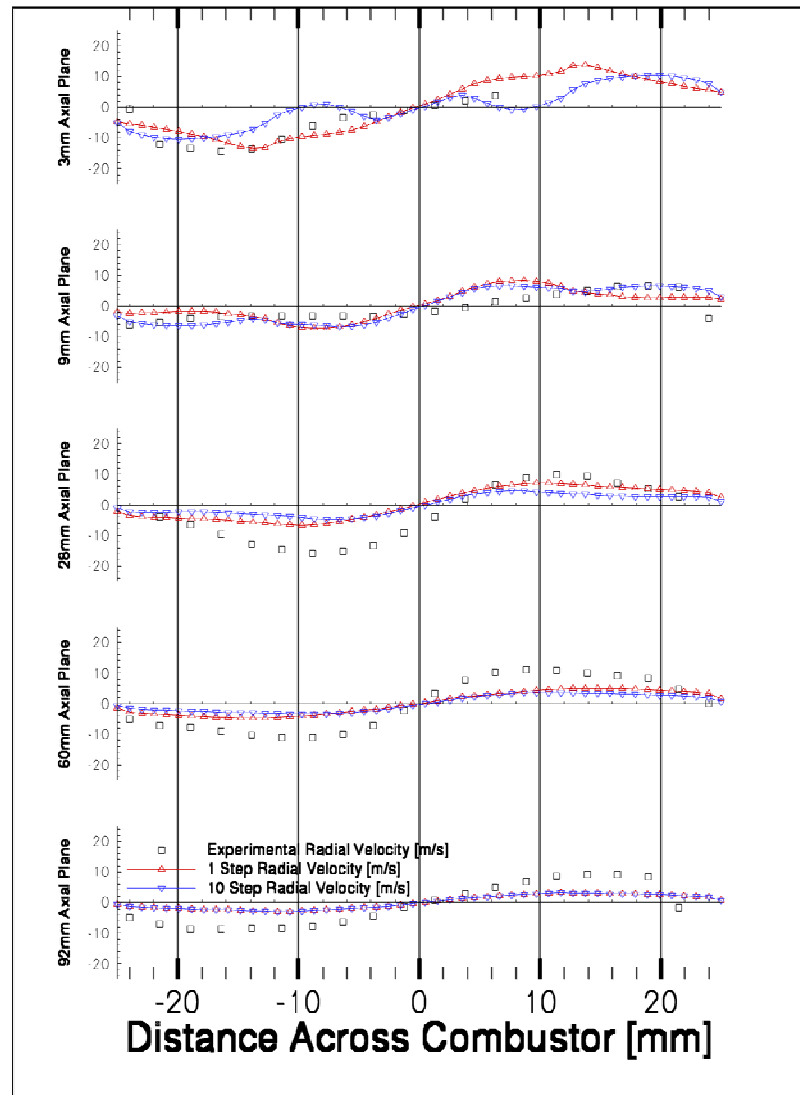


# Reacting Spray Flow, Comparison of Axial Velocity at Various Axial Planes (3, 9, 28, 60, 92mm)



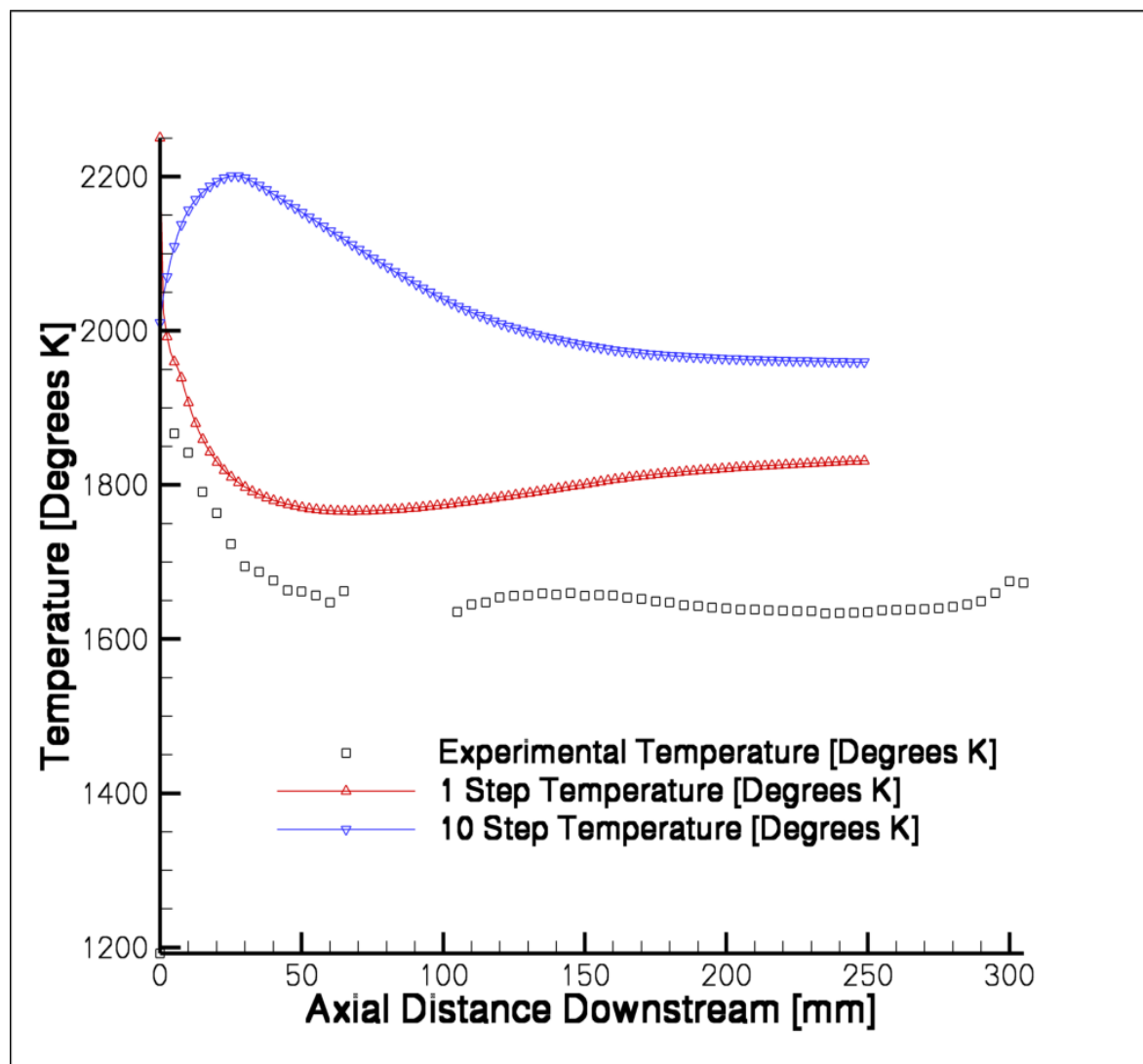


# Reacting Spray Flow, Comparison of Radial Velocity at Various Axial Planes (3, 9, 28, 60, 92mm)



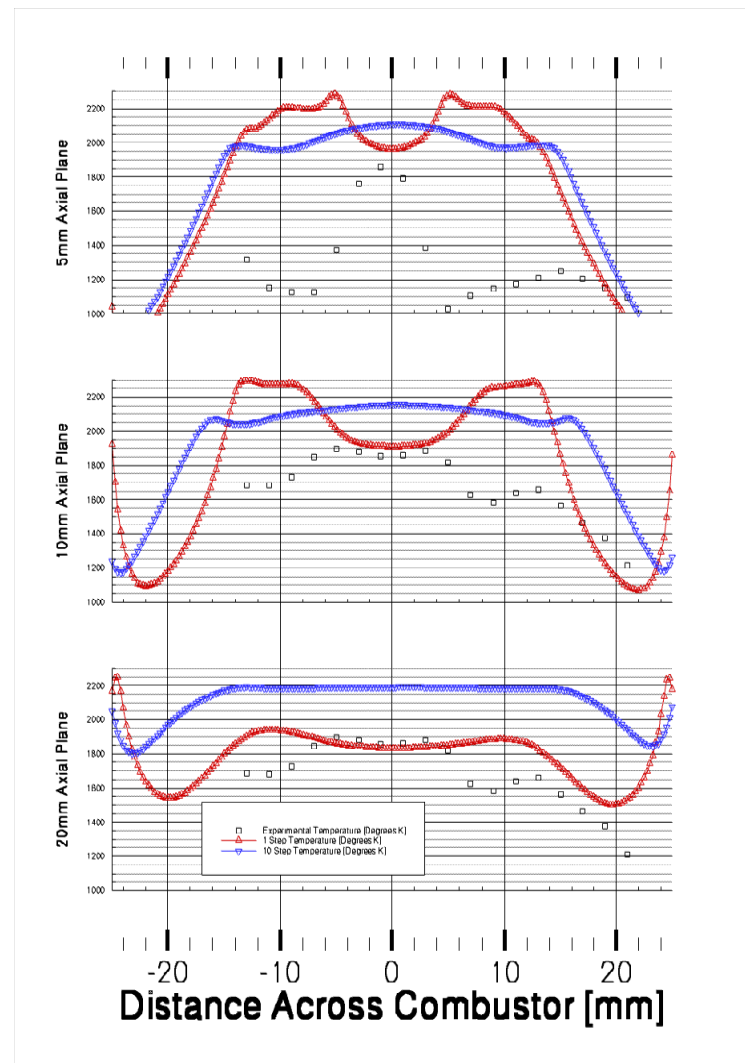


# Reacting Spray Flow, Comparison of Temperature Along the Axial Centerline



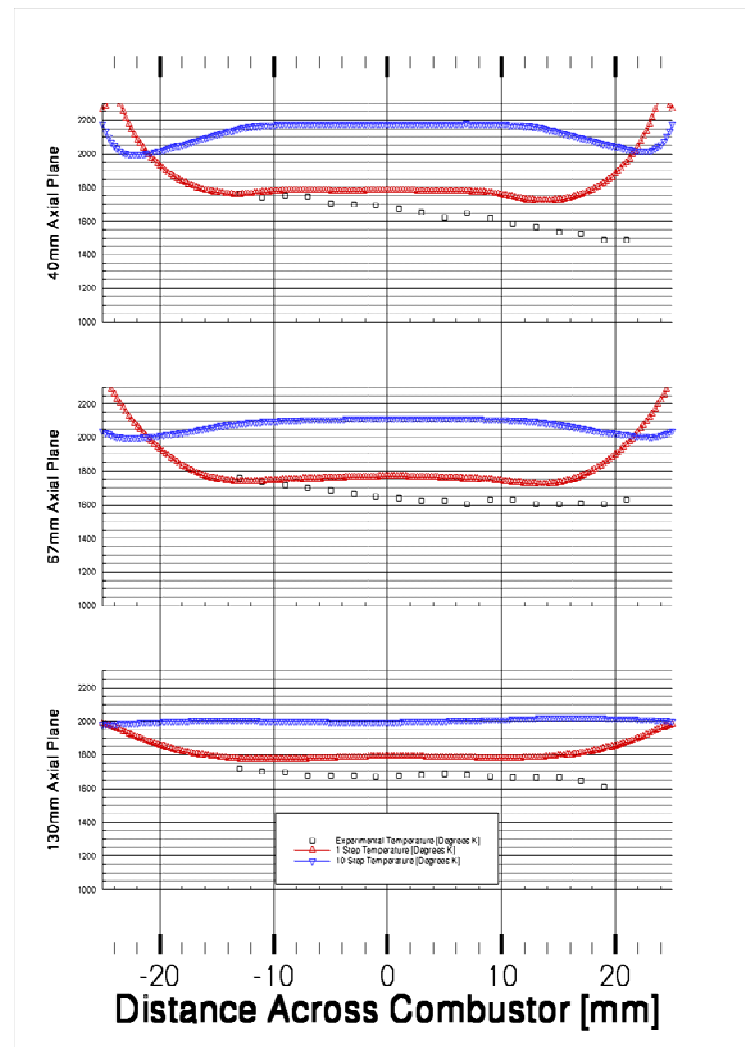


# Reacting Spray Flow, Comparison of Temperature at Various Axial Planes (5, 10, 20mm)



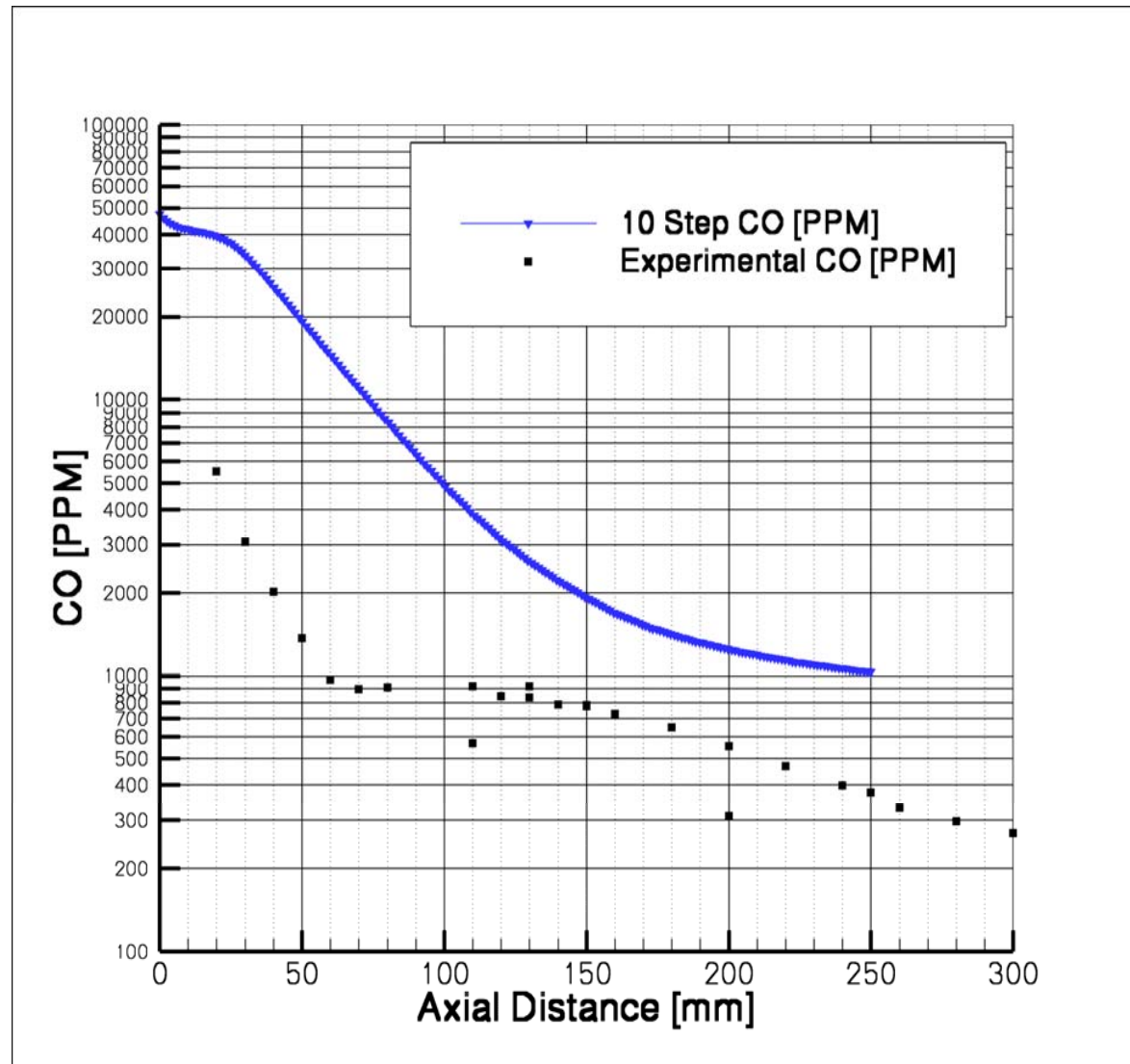


# Reacting Spray Flow, Comparison of Temperature at Various Axial Planes (40, 57, 130mm)



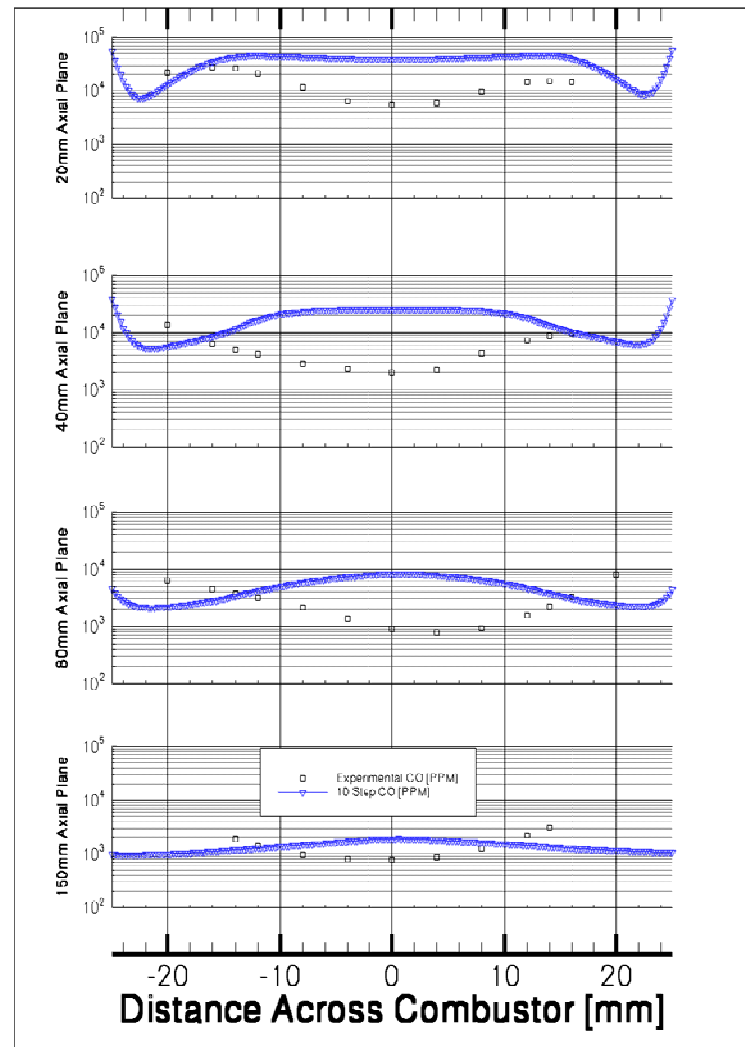


# Reacting Spray Flow, Comparison of CO Along the Axial Centerline



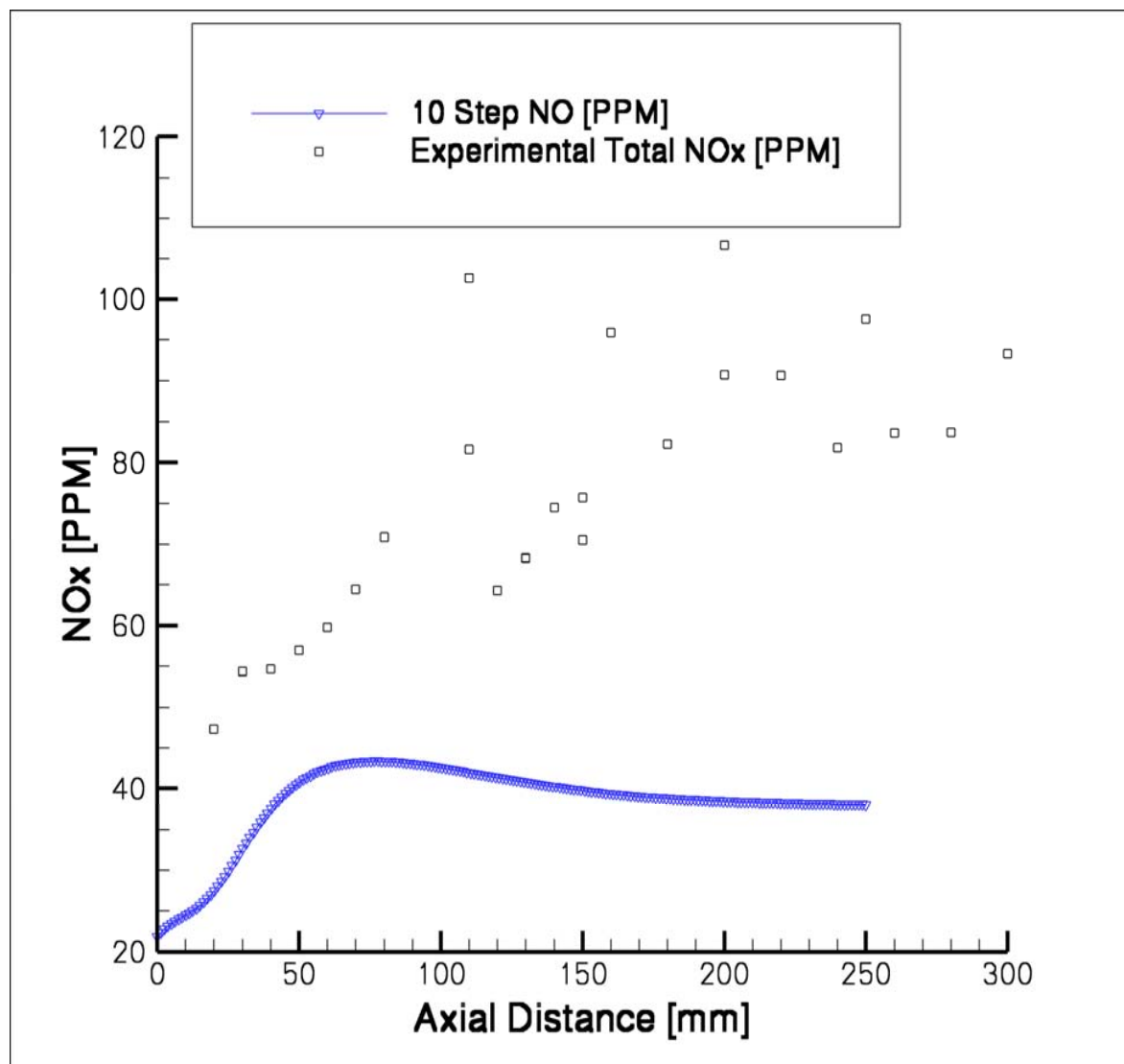


# Reacting Spray Flow, Comparison of CO at Various Axial Planes (20, 40, 80, 150mm)





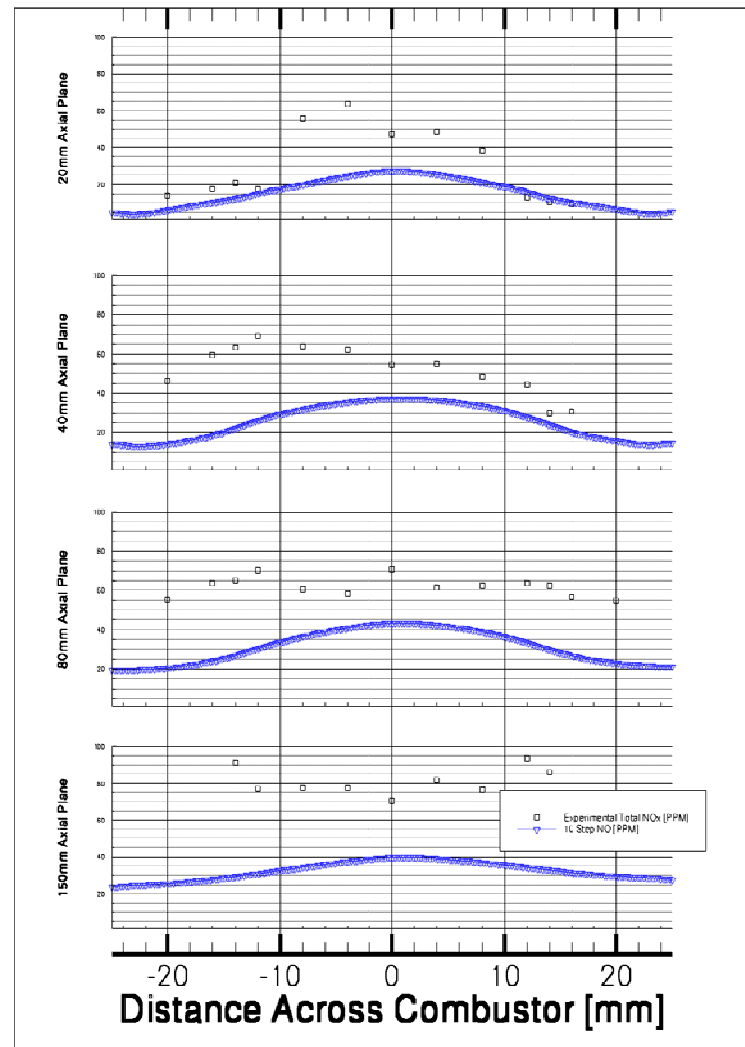
# Reacting Spray Flow, Comparison of $\text{NO}_x$ Along the Axial Centerline





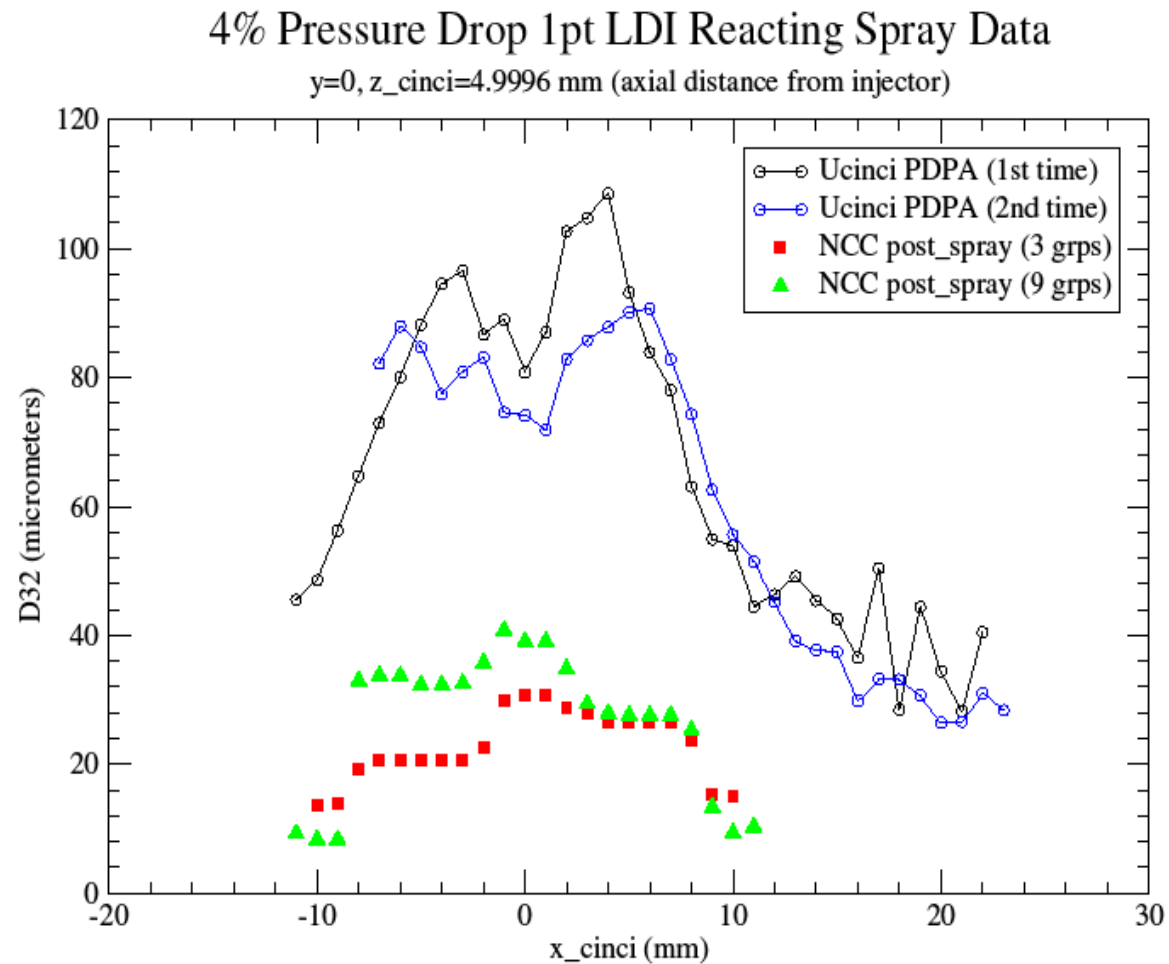


# Reacting Spray Flow, Comparison of $\text{NO}_x$ at Various Axial Planes (20, 40, 80, 150mm)





# Reacting Spray Flow, Sauter Mean Diameter (SMD) Comparison (D32) at a Radial Line





## Partially Resolved Numerical Simulation

- The transient, very large structures of turbulence is computationally captured instead of modeling them all. The computational cost is comparable to that of unsteady RANS simulations.
- The approach is based on temporal filtering with constant filter width which regulates the content of intrinsically unresolved scales. In practice, a resolution control parameter, which is a function of the temporal filter width, is used for this purpose.
- The model for the effects of the unresolved scales is evolved from the state-of-the-art models used in the RANS approach.



## Partially Resolved Numerical Simulation

- In addition to eddy viscosity, the subscale model also accounts for the effects of anisotropy and rotation. Resolution control parameter, unresolved turbulent kinetic energy, and unresolved dissipation rate are needed to close this model.
- Some guidelines

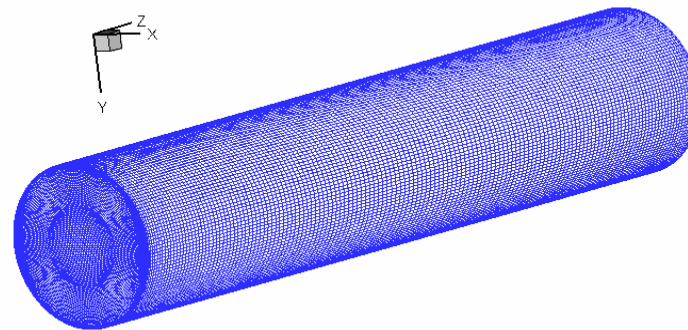
$$RCP \geq \left( \frac{\Delta}{\ell_{RANS}} \right)^{4/3} \left( \frac{k}{k_{RANS}} \right)^{-2}$$

$$N_{PRNS} \geq N_{RANS} \cdot \left( \Delta_{RANS} / \ell_{RANS} \right)^3 \cdot Rcp^{-9/4} \left( k / k_{RANS} \right)^{-9/2}$$



## Simulations of Fully Developed Turbulent Pipe Flow

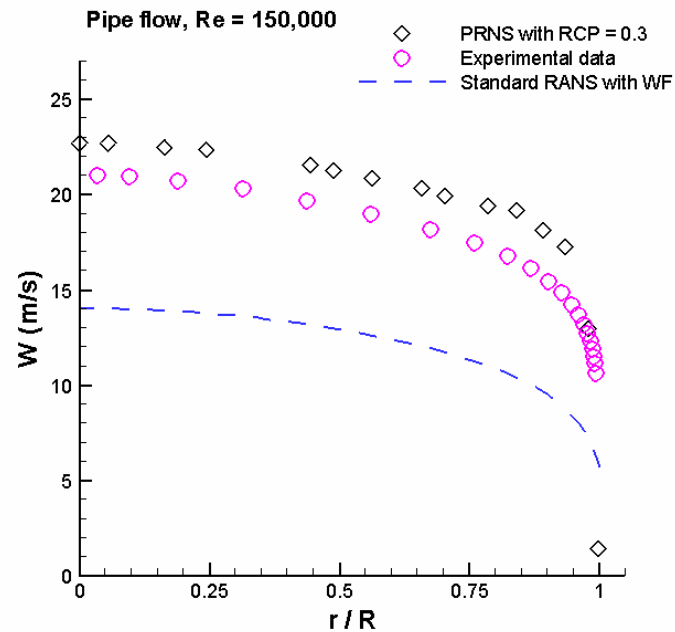
- To assess the effects of RCP, Reynolds number, anisotropy and rotation, and grid size



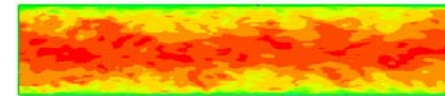
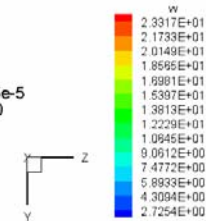
Diameter: 0.12936 m, Length: 5 diameters,  
900705 hexahedra elements



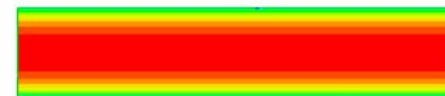
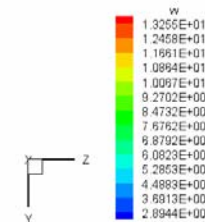
# Fully Developed Turbulent Pipe Flow ( $Re=150,000$ )



PRNS,  $R_{cp}=0.3$   
 $Re=150000$ , 36400 time steps  
 NCC-1.1.4, no smoothing  
 P-reference=100290  
 $2nc=0.0$ , 4th=0.001, CFL=1.0,  $dt=2.5e-5$   
 Convergence 3 order or Max iter=120

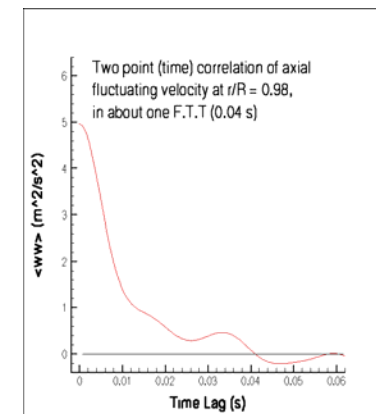
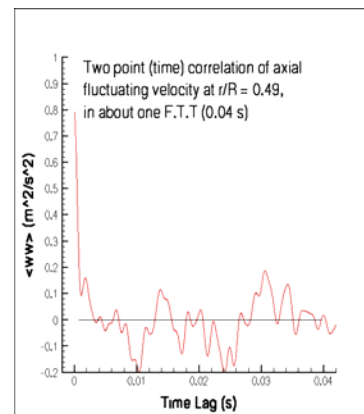
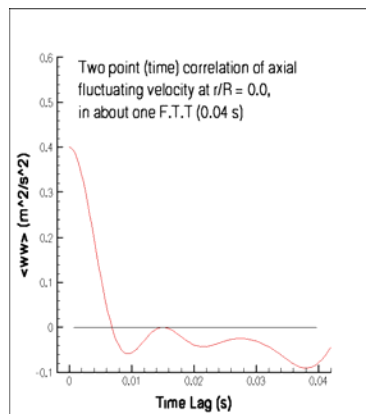
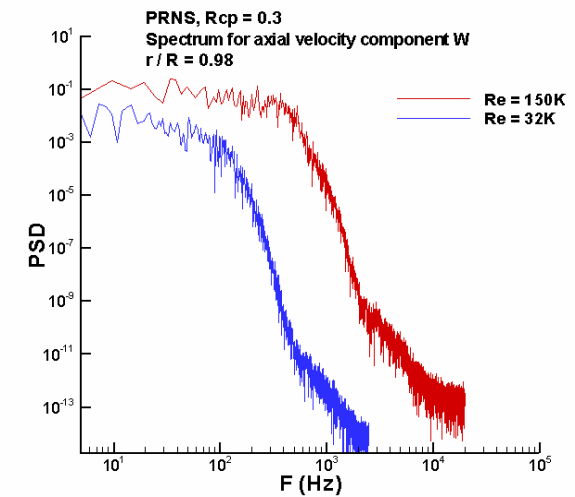
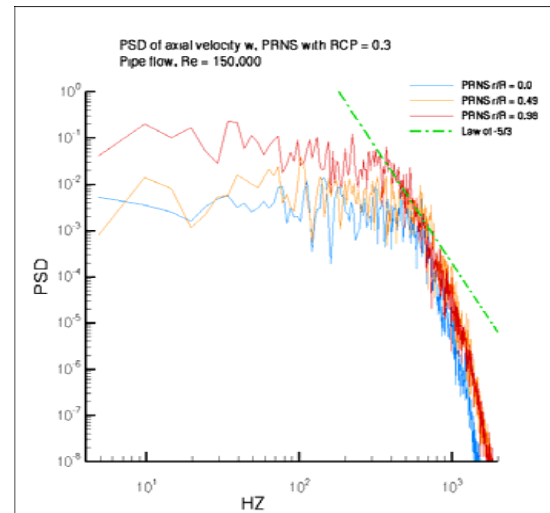
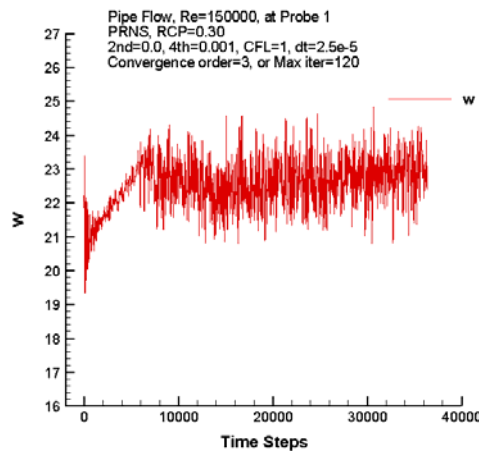


Steady RANS with WF  
 $Re=150000$ , iterations: 400000  
 NCC-1.1.4, no smoothing  
 P-reference=100290  
 $2nd=0.01$ , 4th=0.05, CFL=3.0.





# Fully Developed Turbulent Pipe Flow ( $Re=150,000$ )





# Assessment of NCC for Emissions and Flow Field

## Future Plan

- Complete current assessment tasks.
- Perform steady RANS reacting spray calculations for single LDI element experiment using fuel primary atomization and secondary breakup models.
- Perform non-reacting VLES calculations for single LDI element experiment using the PRNS approach.
- Perform VLES/PRNS reacting spray calculations for single LDI element experiment using fuel primary and secondary breakup models.
- Embark on systematic validation and uncertainty quantification of NCC for emissions and flow fields.
- Conduct reacting flow calculations for SE-5 and CE-5 experiments.
- Assess LES codes from NRA partners.